

Photochemical transformations of 5-methyltetrazole. Matrix isolation FTIR and DFT studies.

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Streszczenie

In situ photolysis of 5-methyltetrazole (MT) isolated in low temperature argon matrices was induced by tunable UV laser radiation. The progress of the reactions was followed by FTIR spectroscopy that allowed for spectroscopic identification of three photoproducts resulting from the MT ring cleavage, namely C-methylnitrilimine CH_3CNNH , N-methylcarbodiimide CH_3NCNH , methylcyanamide CH_3NHCN . The kinetic profiles obtained for these products show different behavior of the species in the course of irradiation. The N-methylcarbodiimide molecules were found to decompose further into two HCN or HNC molecules that interact in the matrix cages to form different hydrogen bonded dimers. Interpretation of the observed photoprocesses was supported by quantum chemical calculations (DFT, TD-DFT).

Słowa kluczowe

Tetrazole ring cleavage, Tunable laser photochemistry,
Methylcarbodiimide, Methylnitrilimine, Methylcyanamide,
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